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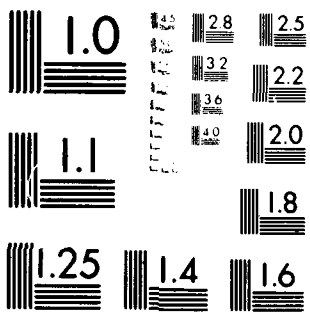

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HEAT CONDUCTION IN FINITE CYLINDERS AND THE COMPUTER-AIDED CALCULATION OF BACTERIA SURVIVAL IN HEAT STERILIZATION

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1. INTRODUCTION

The temperature distribution T(x,y,z,t) in a specimen during heating and cooling of its outer surface is determined by solving the heat diffusion equation for given boundary conditions. Solutions are often obtained for special forms, such as infinite cylinders or infinite slabs, of the specimen, and for some simplified boundary conditions, such as abrupt initial temperature change at the surface of the sample. In practical problems, the solutions are often approximated by simple forms of the time temperature relations. For instance, in the case of retorting of food, the center temperature in the can is usually approximated by a zero order Bessel function valid for very large values of time. Such approximations, while valuable, are inadequate for exact studies. Using modern computers, we were able to calculate T(x,y,z,t) very accurately for any practical size cylinder and for different boundary conditions corresponding to Nusselt numbers between 0 and 5000. The high accuracy and the rapid calculations make the method very useful in many fields of thermal engineering. In the present paper, ~~we apply~~ this method ~~to~~ is used in exact integral calculations of the survival fraction of bacteria during heat sterilization process.

2. HEAT DIFFUSION EQUATION FOR A FINITE CYLINDER

The conduction of heat in a cylinder is given by a second order differential equation. In cylindrical coordinates it is:

$$\frac{\partial T(r, \theta, z, t)}{\partial t} = \kappa \nabla^2 T(r, \theta, z, t) \qquad (1)$$

where $T(r, \theta, z, t)$ is the temperature at point $P(r, \theta, z)$ and at time t, and κ is the thermal diffusivity of the material of the solid

$$\kappa = \frac{\lambda}{\rho \cdot c} = \frac{\text{thermal conductivity}}{\text{density} \cdot \text{specific heat}} \tag{2}$$

We will consider heating a cylindrical specimen from an initial temperature T_i with a constant temperature T_h on the outside of the surface. Then the temperature $T(r, \theta, z, t)$ at any point in the specimen at any time t will be given by Eq. (1), together with the boundary conditions. To simplify the equations, we introduce a new temperature variable:

$$T = T - T_h \tag{3}$$

Eq. (1) becomes

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T \text{ for } r \leq a, \ |z| \leq \ell \tag{4}$$

where a is the radius, and ℓ the half-length of the cylinder. The initial value of T at any point of the specimen is:

$$T_i = T_i - T_h, \text{ for } t \leq o \tag{5}$$

We will consider here the case of convective heating outside the cylinder. At the boundary there will be an interface or transition layer in which the temperature is changing from T_h to the actual temperature of the specimen at the surface. We then obtain the following boundary conditions by equating the heat flowing through the transition layer and the heat flowing through the outermost layer of the specimen.

$$\frac{\partial T}{\partial r} + \frac{h}{\lambda} T = o \text{ at } r = a \tag{6}$$

$$\frac{\partial T}{\partial z} + \frac{h}{\lambda} T = o \text{ at } z = \ell \tag{7}$$

$$\frac{-\partial T}{\partial z} + \frac{h}{\lambda} T = o \text{ at } z = -\ell \tag{8}$$

where λ is conductivity of the specimen, and $h = \lambda gas/\delta gas$, the conductivity of the gas (air) divided by the thickness of the gas (air) film, is the coefficient of heat transfer due to the gas film only.

Due to radiation at the surface, h actually would be equal to λgas/δgas plus some constant. Also, in the case of a meat sample with casing, we have two transition layers instead of one at the surface, the solid casing material and the gas film adhered onto it. All these three factors can be combined into a single coefficient in front of T in Eqs. (6), (7) and (8). Henceforth, h/λ in Eqs. (6), (7) and (8) will stand for this effective coefficient.

Eq. (4) with boundary conditions Eqs. (6) - (8), i.e., $\partial T/\partial r$ being proportional to T, can be solved with the usual technique of the separation of variables.[1,2] The solution for the temperature distribution in a finite cylinder, in our case, takes the following form:

$$T = \sum_j \sum_n A_{j,n} \cdot \cos(\lambda_j z) \cdot J_o(\alpha_n r) \cdot e^{-\kappa(\lambda_j^2 + \alpha_n^2)t} \tag{9}$$

where $A_{j,n}$ are the coefficients of expansion and where $x_n = a \cdot \alpha_n$ are the roots of the following equation (J_o and J_1 being Bessel functions of order zero and one respectively),

$$x_n \cdot J_1(x_n) = \frac{h}{\lambda} a \cdot J_o(x_n) \tag{10}$$

and $y_j = \lambda_j \ell$ are the roots of

$$\frac{h\ell}{\lambda} \cos y_j - y_j \sin y_j = o \tag{11}$$

We have deduced from the boundary conditions the coefficients of expansion $A_{j,n}$ in Eq. (9). After some lengthy calculation, $A_{j,n}$ are found to be

$$A_{j,n} = 2T_i \frac{1}{x_n\left[\left(\frac{x_n}{\nu}\right)^2 + 1\right] \cdot J_1(x_n)} \cdot \frac{4 \sin y_j}{\sin(2 y_j) + 2 y_j} \tag{12}$$

The temperature $T = T(r, \theta, z, t)$ of the specimen is then

$$T - T_h = 2(T_i - T_h) \sum_{j=1}^{\infty} \sum_{n=1}^{\infty} \frac{1}{x_n\left[\left(\frac{x_n}{\nu}\right)^2 + 1\right] \cdot J_1(x_n)} \cdot J_o(\alpha_n r) \cdot \frac{4 \sin y_j}{\sin(2 y_j) + 2 y_j} \cdot \cos \lambda_j z \cdot e^{-\kappa(\lambda_j^2 + \alpha_n^2)t} \tag{13}$$

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where

$$\nu = \frac{h}{\lambda} \cdot a = \text{effective conduction Nusselt Number, or Biot Number}^{(3)} \tag{14}$$

and x_n and y_i are roots of Eqs. (10) and (11).

3. CALCULATIONS OF THE TEMPERATURE DISTRIBUTION

The temperature distribution $T(r, \theta, z, t)$ can be computed for any point $P(r, \theta, z)$ inside the cylinder and any time t provided the roots x_n of Eq. (1) for a given ν, and the roots y_i of Eq. (11) for a given value of $h\ell/\lambda$ are known.

Our task then is to devise first some means to compute rapidly these roots with any practical values of ν and $h\ell/\lambda$.

We have written computer programs which enable us to compute the first 36 roots of Eqs. (10) and (11), for $\nu = 0$ to 5000 and $h\ell/\lambda = 0$ to 10,000, with rapid convergence.

Likewise, the double summation of Eq. (13) has been carried out with the computer. This double summation in principle could be carried out to as many terms as we wish, so long as the values of the roots x_n and y_i are available.

We have also used a temperature variable Ψ, the "relative excess temperature", which is independent of the actual initial and heating temperature,

$$\Psi = \frac{T - T_h}{T_i - T_h} \tag{15}$$

It is seen from Eq. (13) that Ψ is equal to twice the double summation of that equation, and is independent of T_i and T_h. Thus, the actual temperature distributions $T(r, \theta, z, t)$, due to different initial and heating temperatures, can be directly compared or derived from one another.

The temperature distribution $T(r, \theta, z, t)$ in specimens during heating and cooling has often been obtained by some approximations for the heat diffusion equation or its solution. In the present paper we deduced, on the other hand, the exact analytical solution to the heat diffusion equation for finite cylinders in convective heating. The truncation of the two series in Eq. (13) to 36 terms in each of

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the summations results in a very accurate form, allowing $T(r, \theta, z, t)$ to be calculated for any practical size finite cylinders and for Nusselt (Biot) number extending from 0 to 5000. The method developed should have great applicability in thermal engineering industry. Tables I - II give the relative excess temperature Ψ on the cross sections at $z/\ell = 0$, and 0.6 respectively, at $r/a = 0, 0.2, 0.4,$-- 1.0 and times t = 5, 10, 15,---240 minutes, for a specimen of radius $a = 5$ cm, half-length $\ell = 2.5$ cm, with $\kappa = 1.35 \times 10^{-3}$ cm^2s^{-1} and $\nu = 6.0$. Similar tables for Ψ on the cross sections $z/\ell = 0.2, 0.4, 0.8$, and 1.0, are available from the authors.

The last columns of these tables give the survival fraction calculations of bacteria during sterilization to be discussed in later sections.

Figs. la-lf are the computer plots of these tables.

4. CALCULATION OF BACTERIA SURVIVAL IN HEAT STERILIZATION

We now apply the above calculations of heat diffusion to thermal killing of bacteria in finite cylindrical specimens. The microbial kill is described quantitatively by the survival fraction N/N_o where N is the number of bacteria survived at time t and N_o is the initial value of N. For a large class of microorganisms, N/N_o during thermal sterilization at a given constant temperature T follows closely the following equation [1,5,6]:

$$\ell n \frac{N}{N_o} = -C \cdot [\exp(-E_a/RT)] \cdot t \qquad (16)$$

where

E_a = the Arrhenius activation energy in kcal-mol^{-1} for inactivating a unit or a molecule that is essential for the survival of a bacterium

R = the universal gas constant in J·mol^{-1}

T = sterilization temperature in Kelvin

t = sterilization time in s

C = a constant

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TABLES I & II- RELATIVE TEMPERATURE DIFFERENCES, $\psi = (T - T_h)/(T_i - T_h)$ IN TWO CROSS SECTIONS AT $Z/\ell = 0$ AND 0.6. THE FIRST COLUMN GIVES THE TIME, THE COLUMNS 2-7 GIVE ψ FOR DIFFERENT DISTANCES r/a 0, 0.2, 0.4, 0.6, 0.8, 1.0 AND COLUMN 8 GIVES THE SURVIVAL FRACTION FOR Cl. BOTULINUM SPORES AT r/a = 0.

TABLE I

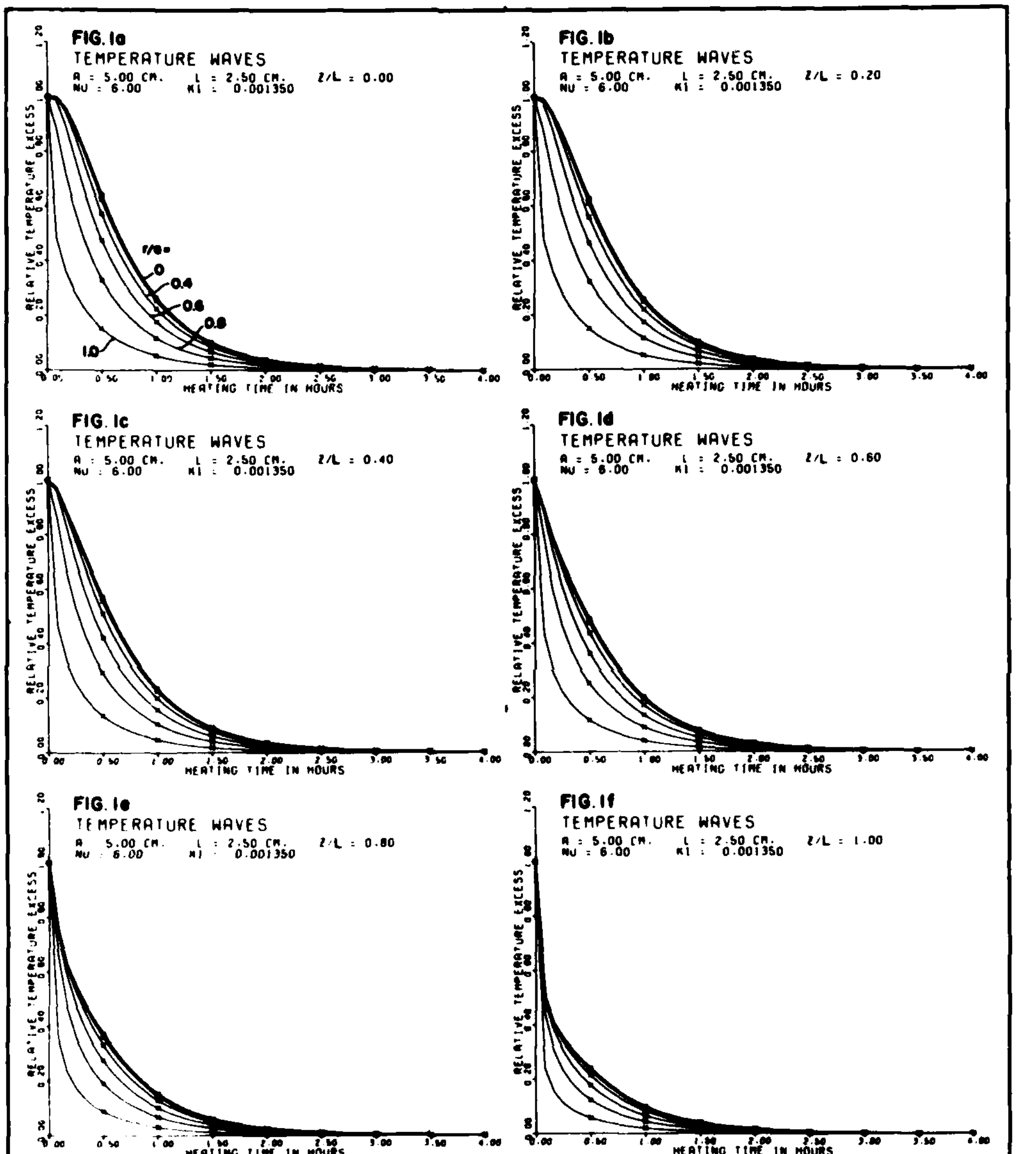
A = 5.0 CM L = 2.5 CM Z/L = .0
NU = 6.0 K1 = 1.35-03 CM SQ/S

TIME	DISTANCE FROM AXIS						S F
MIN	0.0	0.2	0.4	0.6	0.8	1.0	AT AXIS
5	.9973	.9973	.9970	.9876	.8853	.4809	1.000+00
10	.9627	.9618	.9528	.9015	.7252	.3632	1.000+00
15	.8972	.8921	.8656	.7814	.5906	.2855	1.000+00
20	.8168	.8089	.7644	.6649	.4833	.2290	1.000+00
25	.7297	.7154	.6652	.5628	.3984	.1863	1.000+00
30	.6436	.6274	.5744	.4761	.3307	.1533	1.000+00
35	.5623	.5457	.4937	.4031	.2763	.1272	1.000+00
40	.4879	.4719	.4233	.3417	.2319	.1062	9.999-01
45	.4212	.4064	.3622	.2900	.1953	.0892	9.991-01
50	.3620	.3490	.3096	.2463	.1650	.0752	9.961-01
55	.3109	.2991	.2643	.2094	.1397	.0635	9.789-01
60	.2663	.2559	.2256	.1781	.1185	.0538	9.200-01
65	.2277	.2187	.1924	.1516	.1006	.0456	7.968-01
70	.1946	.1868	.1641	.1290	.0855	.0387	5.576-01
75	.1661	.1594	.1399	.1099	.0727	.0329	2.665-01
80	.1417	.1360	.1193	.0936	.0619	.0280	[illegible]
85	.1209	.1159	.1016	.0797	.0527	.0238	6.851-03
90	.1031	.0989	.0866	.0679	.0448	.0203	1.930-04
95	.0879	.0843	.0738	.0578	.0382	.0173	1.896-06
100	.0749	.0718	.0629	.0493	.0325	.0147	4.860-10
105	.0639	.0612	.0536	.0420	.0277	.0125	8.467-14
110	.0544	.0522	.0457	.0357	.0236	.0107	7.410-19
115	.0464	.0444	.0389	.0305	.0201	.0091	5.456-25
120	.0395	.0379	.0332	.0259	.0171	.0077	3.249-32
125	.0337	.0323	.0283	.0221	.0146	.0066	0.000
130	.0287	.0275	.0241	.0188	.0124	.0056	0.000
135	.0244	.0234	.0205	.0160	.0106	.0048	0.000
140	.0208	.0200	.0175	.0137	.0090	.0041	0.000
145	.0177	.0170	.0149	.0116	.0077	.0035	0.000
150	.0151	.0145	.0127	.0099	.0065	.0030	0.000
155	.0129	.0123	.0108	.0085	.0056	.0025	0.000
160	.0110	.0105	.0092	.0072	.0048	.0021	0.000
165	.0094	.0090	.0078	.0061	.0040	.0018	0.000
170	.0080	.0076	.0067	.0052	.0034	.0016	0.000
175	.0068	.0065	.0057	.0045	.0029	.0013	0.000
180	.0058	.0055	.0049	.0038	.0025	.0011	0.000
185	.0049	.0047	.0041	.0032	.0021	.0010	0.000
190	.0042	.0040	.0035	.0028	.0018	.0008	0.000
195	.0036	.0034	.0030	.0023	.0015	.0007	0.000
200	.0030	.0029	.0026	.0020	.0013	.0006	0.000
205	.0026	.0025	.0022	.0017	.0011	.0005	0.000
210	.0022	.0021	.0019	.0015	.0010	.0004	0.000
215	.0019	.0018	.0016	.0012	.0008	.0004	0.000
220	.0016	.0015	.0013	.0011	.0007	.0003	0.000
225	.0014	.0013	.0011	.0009	.0006	.0003	0.000
230	.0012	.0011	.0010	.0008	.0005	.0002	0.000
235	.0010	.0010	.0008	.0007	.0004	.0002	0.000
240	.0008	.0008	.0007	.0006	.0004	.0002	0.000

TABLE II

A = 5.0 CM L = 2.5 CM Z/L = .6
NU = 6.0 K1 = 1.35-03 CM SQ/S

TIME	DISTANCE FROM AXIS						S F
MIN	0.0	0.2	0.4	0.6	0.8	1.0	AT AXIS
5	.9027	.9027	.9024	.8939	.8013	.4353	1.000+00
10	.7881	.7874	.7808	.7380	.5937	.2974	1.000+00
15	.7013	.6973	.6766	.6107	.4616	.2232	1.000+00
20	.6258	.6175	.5866	.5094	.3703	.1794	1.000+00
25	.5543	.5434	.5053	.4275	.3026	.1415	1.000+00
30	.4871	.4748	.4347	.3603	.2503	.1160	9.999-01
35	.4249	.4124	.3731	.3046	.2088	.0961	9.991-01
40	.3685	.3564	.3196	.2580	.1751	.0802	9.957-01
45	.3180	.3068	.2734	.2189	.1475	.0673	9.820-01
50	.2735	.2635	.2337	.1859	.1246	.0567	9.382-01
55	.2347	.2258	.1995	.1581	.1055	.0479	8.264-01
60	.2010	.1932	.1703	.1345	.0894	.0406	6.090-01
65	.1719	.1651	.1453	.1144	.0759	.0344	3.217-01
70	.1469	.1410	.1239	.0974	.0645	.0292	9.662-02
75	.1254	.1203	.1056	.0829	.0549	.0249	1.236-02
80	.1070	.1026	.0900	.0706	.0467	.0211	[illegible]
85	.0913	.0875	.0767	.0601	.0397	.0180	4.101-06
90	.0778	.0746	.0654	.0512	.0338	.0153	5.482-09
95	.0663	.0636	.0557	.0436	.0288	.0130	8.787-13
100	.0565	.0542	.0475	.0372	.0245	.0111	1.376-17
105	.0482	.0462	.0405	.0317	.0209	.0095	1.848-23
110	.0411	.0394	.0345	.0270	.0178	.0080	2.010-30
115	.0350	.0335	.0294	.0230	.0152	.0069	1.817-38
120	.0298	.0286	.0250	.0196	.0129	.0058	0.000
125	.0254	.0244	.0213	.0167	.0110	.0050	0.000
130	.0217	.0208	.0182	.0142	.0094	.0042	0.000
135	.0184	.0177	.0155	.0121	.0080	.0036	0.000
140	.0157	.0151	.0132	.0103	.0068	.0031	0.000
145	.0134	.0128	.0112	.0088	.0058	.0026	0.000
150	.0114	.0109	.0096	.0075	.0049	.0022	0.000
155	.0097	.0093	.0082	.0064	.0042	.0019	0.000
160	.0083	.0079	.0070	.0054	.0036	.0016	0.000
165	.0071	.0068	.0059	.0046	.0031	.0014	0.000
170	.0060	.0058	.0050	.0039	.0026	.0012	0.000
175	.0051	.0049	.0043	.0034	.0022	.0010	0.000
180	.0044	.0042	.0037	.0029	.0019	.0009	0.000
185	.0037	.0036	.0031	.0024	.0016	.0007	0.000
190	.0032	.0030	.0027	.0021	.0014	.0006	0.000
195	.0027	.0026	.0023	.0018	.0012	.0005	0.000
200	.0023	.0022	.0019	.0015	.0010	.0005	0.000
205	.0020	.0019	.0016	.0013	.0008	.0004	0.000
210	.0017	.0016	.0014	.0011	.0007	.0003	0.000
215	.0014	.0014	.0012	.0009	.0006	.0003	0.000
220	.0012	.0012	.0010	.0008	.0005	.0002	0.000
225	.0010	.0010	.0009	.0007	.0004	.0002	0.000
230	.0009	.0008	.0007	.0006	.0004	.0002	0.000
235	.0007	.0007	.0006	.0005	.0003	.0001	0.000
240	.0006	.0006	.0005	.0004	.0003	.0001	0.000



FIGS. 1a-1f-THE ORDINATE SHOWS THE RELATIVE TEMPERATURE DIFFERENCES, $\psi = (T-T_h) / (T_i-T_h)$, IN A FINITE CYLINDER FOR VARIOUS CROSS SECTIONS AT Z/ℓ EQUAL 0, 0.2, 0.4, 0.6, 0.8, 1.0. THE ABSCISSA SHOWS THE HEATING TIME t.

(391)

In this case where T is constant, we obtain by differentiation of Eq. (16), that the kill rate function (dN/dt)/N is the exponential exp $(-E_a/RT)$, that is:

$$\frac{dN}{dt} \cdot \frac{1}{N} = -C \cdot [\exp(-E_a/RT)] = -C \cdot F(T(t),\ t) \tag{17}$$

In some experiments it is found that the semi-logarithmic plot of the survival fraction has a "shoulder". This may be represented by the function

$$F(T(t),t) = 1 - [1-\exp(-E_a/RT(t))]^n \tag{18}$$

which for n = 1 reduces to the form in Eq. (17), the frequently used Arrhenius function:

$$F(T(t),\ t) = \exp\ [-E_a/RT(t)] \tag{19}$$

We now show that for the general case where the kill rate function assumes a general form F(T(t), t), with the temperature T(t) varying with time t, the survival fraction is given by the following time integral:

$$\ell n\ \frac{N}{N_o} = -C \int_o^t F(T(t),\ t)\ dt \tag{20}$$

From the emperical law Eq. (16) for constant T,

$$\ell n\ \frac{N}{N_o} = -C \cdot [\exp(-E_a/RT)] \cdot T \tag{16}$$

we obtain the following differential form in terms of the kill rate

$$\frac{dN}{dt} = -C \cdot [\exp(-E_a/RT)] \cdot N \tag{21}$$

Now we generalize Eq. (21) to include the case where T varies with t. By integrating Eq. (21) for this temperature varying case, we have the following time integral for the logarithmic survival fraction

$$\ell n\ \frac{N}{N_o} = -C \int_o^t \exp\ (-E_a/RT)\ dt \tag{22}$$

(397)

Next, we generalize Eqs. (21) for the general kill rate function F(T(t), t),

$$\frac{dN}{dt} = -C \cdot F(T(t), t) \cdot N \tag{21a}$$

the logarithmic survival fraction is then

$$\log \frac{N}{N_o} = -C \int_o^t F(T(t), t)\, dt \tag{22a}$$

which is Eq. (20).

5. CALCULATIONS OF BACTERIAL SURVIVAL EQUATION

We now put our function T(t) of Eq. (13) into the "bacterial survival integral" of Eqs. (22) or (22a) to calculate the survival fraction N/N_o of the bacterium. In this paper, we carried out the calculations for Cl. botulinum spores for which we assume the kill rate function to be given by the exponential function $\exp(-E_a/RT)$ rather than the general function F(T(t), t) which may represent any empirical function or other theoretical function such as Eyring's.

The calculations for other microorganisms will be exactly the same.

The integrand of Eq. (22) after substituting T from Eq. (13) looks quite complicated. We have written computer programs to carry out the computation. But, before we carry out the computation, the two constants, which characterize the bacterium being considered, C and E_a in Eqs. (16) and (22), have to be determined.

6. DETERMINATION OF E_a

We show in some details below the relationship between the so-called z-value in the terminology used by the microbiologist, the temperature T, and the Arrhenius activation energy E_a.

The reaction rate equation, Eq. (21a),

$$\frac{dN}{dt} = -kN = -C \cdot [\exp(-E_a/RT)] \cdot N \tag{21}$$

means that the temperature dependence of k is through T in the exponential function $\exp(-E_a/RT)$ only where E_a is a constant independent of T. Otherwise, k will have to be expressed by the general function

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$F(T(t), t)$. Thus, at temperatures T_1 and T_2, we have

$$\left(\frac{dN}{dt}\right)_1 = -C\cdot \left[\exp(-E_a/RT_1)\right] \cdot N \quad (23)$$

$$\left(\frac{dN}{dt}\right)_2 = -C\cdot \left[\exp(-E_a/RT_2)\right] \cdot N \quad (24)$$

From Eqs. (23) and (24),

$$\frac{(dN/dt)_1}{(dN/dt)_2} = \exp\left[-\frac{E_a}{R}\,\frac{T_2 - T_1}{T_1 T_2}\right] \quad (25)$$

Now if we choose the temperature T_2 such that the rate of inactivation is changed by a factor of 10 from that at T_1, that is:

$$\frac{(dN/dt)_1}{(dN/dt)_2} = 10 \quad (26)$$

whence, using Eq. (25) it follows that:

$$E_a = \frac{(\ln 10)\cdot R\, T_1 T_2}{T_1 - T_2} \doteq \frac{(\ln 10)\cdot R\, T_1 T_2}{z} \quad (27)$$

where, by definition, $T_1 - T_2$, the temperature change as specified, is the z-value.

In case of Cl. botulinum spores, representative values for z are in the range $z = 10.4 \pm 0.8^o$ at 121.1^oC[4]. From Eq. (27), we have then for Cl. botulinum spores,

$$E_a = \frac{(\ln 10)\cdot 394.26 \cdot 384.26 \cdot 1.987 \cdot 10^{-3}}{10.4}$$
$$= 66.6 \pm 5.4 \text{ kcal. mol}^{-1} \quad (28)$$

7. DETERMINATION OF THE CONSTANT C

For Cl. botulinum spores, we will use for 12D (i.e., reduction of the spore number to 10^{-12} of the initial number) the conservative F_o-value of 3.5 min for non-acid and non-cured meats, which means that heating at 121.1^oC for 17.5 sec. (= 3.5 x 60/12) reduces

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the number N by one order of magnitude. Thus, from Eq. (16), for Cl. botulinum spores,

$$[C \cdot \exp(-E_a/RT)] \cdot 17.5 = \ln 10$$

giving

$$C = \frac{2.3026}{17.5} \cdot e^{85.076}$$

$$= 1.17 \cdot 10^{36} s^{-1}$$

Calculations are made rather simply with the computer of Eq. (22) as a function of time. The last columns of Tables I and II give the values of the survival fraction N/N_o at the axis thus computed. Fig. 2 is the plot of these "integral" survival curves for Cl. botulinum spores at the center of the cross-sectional planes $z/\ell = 0, 0.4, 0.6, 0.8$ and 1.0, of the cylinder with $a = 5$ cm, $\nu = 6$ and $\kappa = 1.35 \times 10^{-3}$ cm^{2}s^{-1}. The heating and the initial temperatures T_h and T_i, are 121.1°C and 21°C respectively.

It is seen from the survival curve for $z = o$ that in order to reduce the survival fraction of Cl. botulinum spores to 10^{-12} of the initial spore number, about 1-1/2 hours heating is needed for a beef roll of radius = 5 cm and 5 cm long.

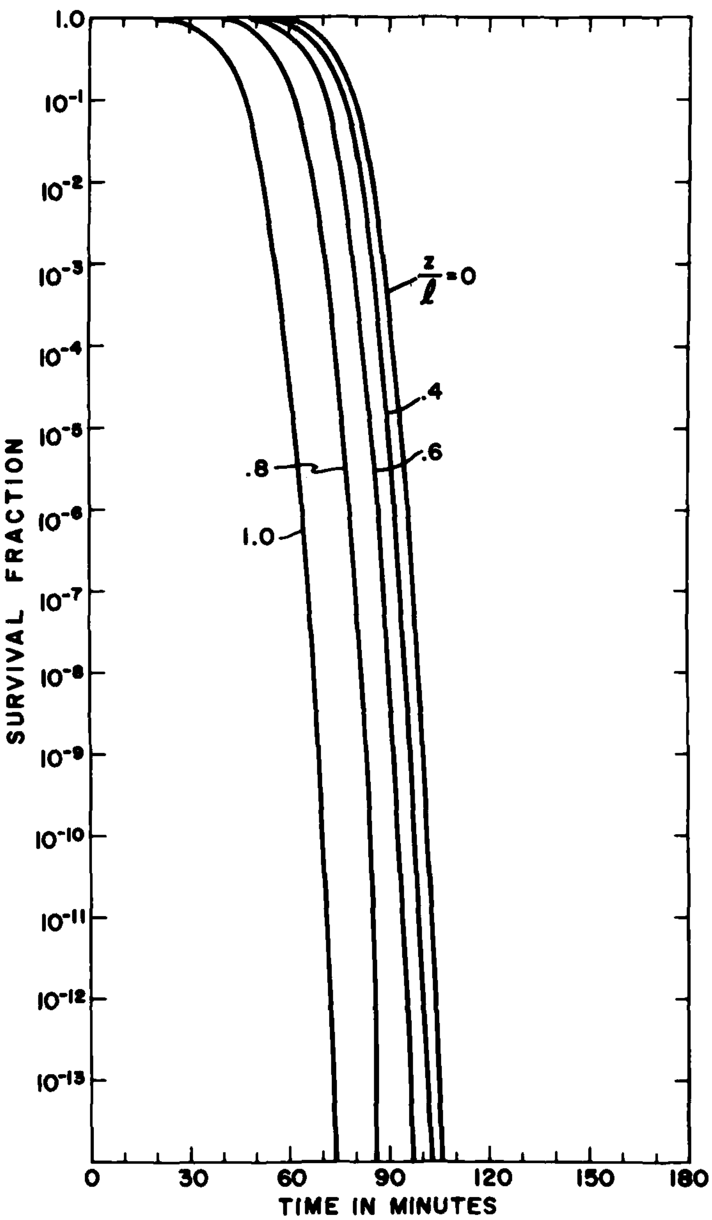

FIG. 2. INTEGRAL SURVIVAL CURVES FOR CL. BOTULINUM SPORES AT THE CENTER ($r/a = 0$) OF THE CROSS SECTIONAL PLANES $z/\ell = 0, 0.4, 0.6, 0.8, 1.0$, OF A FINITE CYLINDER.

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